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Since the discovery of Ti-doped $NaAlH_4$ as a possible candidate for reversible solid state hydrogen storage [1], a lot of effort has been made to investigate and understand the decomposition processes and kinetics of $NaAlH_4$ and Na_3AlH_6, an intermediate product in the desorption processes. Of particular interest is the effect of the Ti-doping on cyclic hydrogen discharging and recharging [2], being essential for mobile hydrogen storage applications.
In this contribution, we present results of density-functional calculations [3] for bulk $NaAlH_4$ and Na_3AlH_6. We have determined activation energies for hydrogen diffusion and rotation of AlH_4^- and AlH_6^{3-} anions, respectively. We furthermore provide results for bulk substitutions of Ti at Al-sites.

[1] Bogdanović, Schwickardi, J. Alloys Compd. 253 (1997)
[2] Bogdanović *et al.*, J. Alloys Compd. 350 (2003)
[3] Dacapo pseudopotential code. URL http://www.camp.dtu.dk/campos
Hammer, Hansen, Nørskov, PRB 59, 7413 (1999)